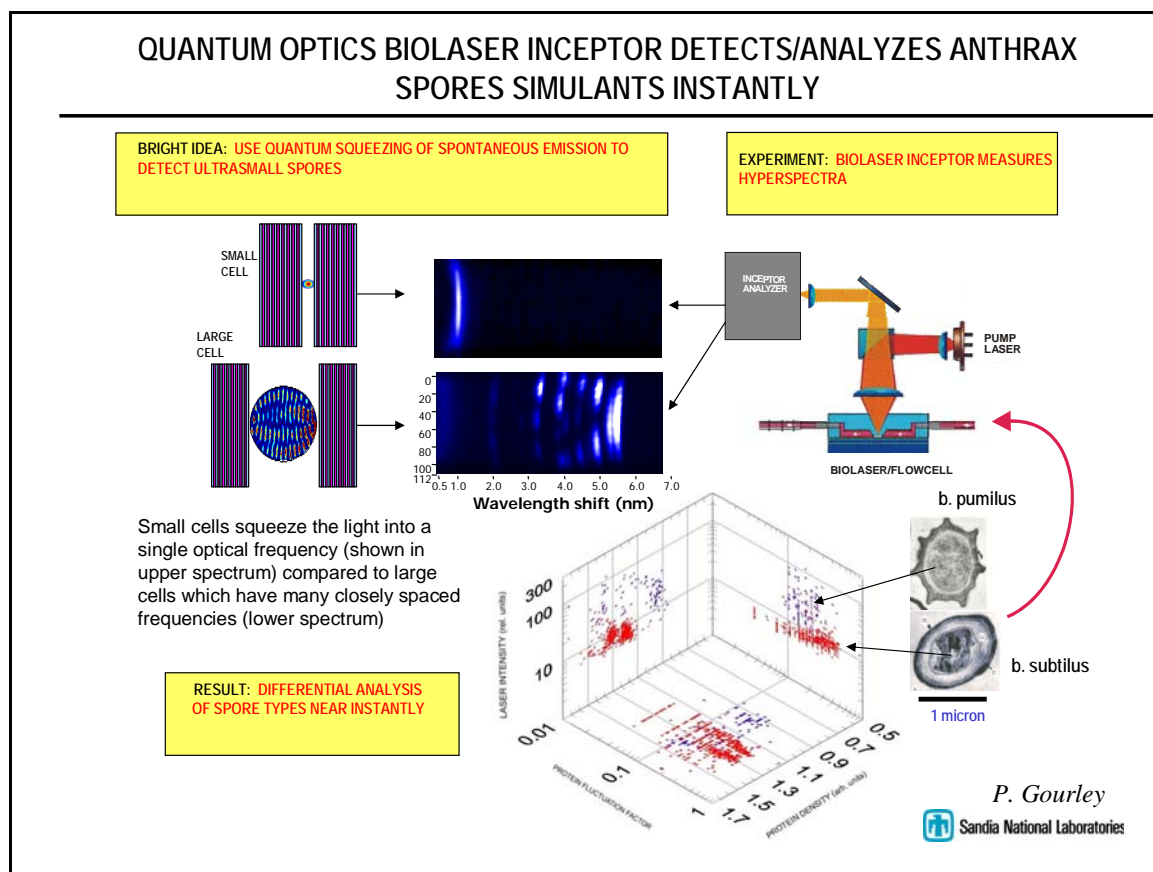


A Biolaser for the Rapid Detection and Analysis of Anthrax Spores

Investigator: P. Gourley, Sandia National Labs.

You return to your office and discover a white powder on the desk next to a recently delivered letter. Is it just powdered creamer spilled from your morning coffee preparation, a carryover from an experiment you are doing down the hall on an innocuous bacteria, or something more sinister associated with the letter (such as anthrax)? A highly sensitive quantum optics device using a biocompatible semiconductor laser microcavity has been shown to be up to the task in tests on spore simulants. This device is based on recent advances in the surface chemistry of semiconductors and the concept of quantum squeezing of light emitted through a spore flowing at high speed in the laser's microcavity. This light squeezing enables even tiny spores to generate a whoppingly large signal which, when analyzed, yields critical biological information including the spore's protein coat morphology, spore shape, intracellular granularity, protein density and uniformity. This field-deployable BioLaser should be able to identify different types of anthrax spores within a population of non-pathogenic spores much more rapidly (minutes) than current cumbersome, slow and expensive methods.

Reference: Biolaser for High-speed Cell Biology, *J. Phys. D* 36, R228 (2003) (invited); special issue on *Biophotonic* (submitted).

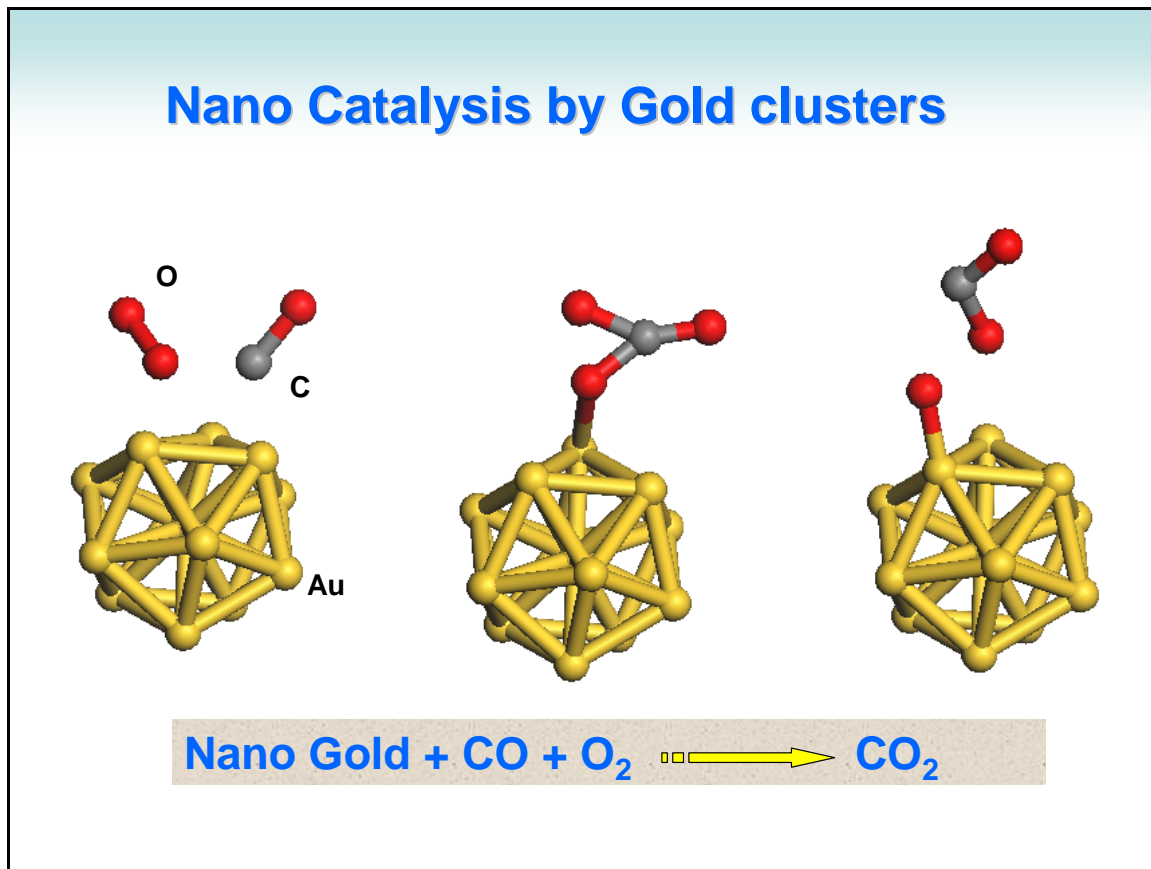


Loss of Nobility of Gold at the Nanoscale

Investigator: P. Jena, Virginia Commonwealth University

Although gold is the noblest of all metals, gold clusters smaller than 3-4 nanometers serve as an efficient catalyst even below room temperature. The existence of oxygen bound in molecular form to anionic gold clusters has now been observed. The stabilization of the di-oxygen species on gold clusters provides a clear pathway for the oxidation of CO; specifically negative gold nano-particles containing molecularly bound oxygen can interact with CO to give rise to an intermediate complex CO_3 , which then decomposes to yield CO_2 . This mechanism may also be responsible for other reactions such as the partial oxidation of propylene. This research demonstrated that the synergy between photoelectron spectroscopy experiments and theoretical determination of structure can provide crucial information for obtaining a molecular level understanding of catalysts consisting of nanomaterials.

Reference: *J. Am. Chem. Soc.* 125, 2848 (2003).



Giant Magnetic Moments of Nitrogen Doped Manganese Clusters

Investigator: P. Jena, Virginia Commonwealth University

Manganese atoms, which otherwise bind weakly and couple antiferromagnetically with each other, were predicted to couple strongly in the presence of nitrogen. In addition, the nitrogen-induced manganese clusters carry giant magnetic moments. For example, an Mn_5N cluster carries a magnetic moment of 22 Bohr magnetons, which is 10 times larger than the magnetic moment per atom of bulk iron, namely 2.2 Bohr magnetons. The prediction that the origin of the frequently observed high temperature ferromagnetism in (Ga, Mn)N layers is related to the formation of Mn-rich clusters is consistent with recently published experimental work. This finding will be useful for the design of new magnetic materials, may play an important role in understanding the large variation in the Curie temperature of other materials, such as Mn-doped GaN, and may impact the design of novel spintronic devices.

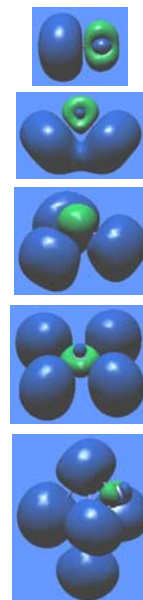
Reference: *Phys. Rev. Lett.* 89, 185504 (2002).

Giant Magnetic Moments from Manganese-Nitrogen Clusters

- Manganese atoms bind weakly. Mn_2 is a van der Waals molecule.
- Mn atoms couple antiferromagnetically.
- In the presence of a nitrogen atom, the binding increases substantially and it becomes ferromagnetic.
- Each Mn atom binds with the N atom antiferromagnetically and all the Mn atoms end up with their spins aligned ferromagnetically.
- It is expected that due to this enhancement of their magnetic moments small clusters of Mn when doped with N may be useable as molecular magnets.
- Applications in spintronics may also be possible.

Note that bulk Mn is nonmagnetic while Mn_5N has a magnetic moment of 22 Bohr magnetons. In comparison, bulk Fe has a magnetic moment of 2.2 Bohr magnetons per atom.

Spin density surfaces for Mn_xN clusters. Green and blue correspond to negative and positive spins.



P. Jena, Virginia Commonwealth University

Two-Dimensional Photonic Band Gap Crystals Based on Self-Assembled Carbon Nanotube Arrays

Investigator: Z. F. Ren, Boston College

Two-dimensional (2D) photonic band gap crystals in the visible wavelength have been fabricated for the first time based on the self-assembled periodic arrays of aligned carbon nanotubes. The fabrication of such unique structures have been extremely challenging due to their required spacing of 400 to 700 nanometers between the one-dimensional (1D) nanocylinders. Such crystals have now been fabricated based on arrays of carbon nanotubes made by self-assembly and plasma-enhanced chemical vapor deposition. These aligned periodic carbon nanotubes are unique in the sense that they interact with white light to show monochromatic colors. The advantages are (1) these crystals exhibit a photonic band gap not previously observed in the visible region, and (2) the feasibility of fabricating large area 2D photonic band gap crystals without expensive electron lithography and ion plasma dry etching has been demonstrated.

Technologically, these arrays not only separate the optical signals with precision, but they also totally reflect certain frequencies. These arrays may find wide applications in optical signal processing on demultiplexing, demodulation, and (optical) switching, etc. This work has been featured in *Nature Materials*, *Nature Materials Update*, *Bulletin of the Materials Research Society*, *Small Times Magazine*, *Materials Today*, *Nanotechweb*, *step gateway*, etc.

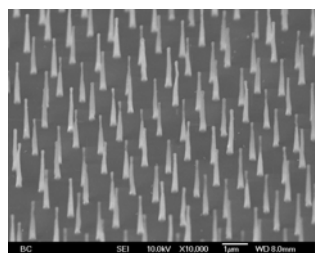
Reference: *NanoLetters* 3, 13 - 18 (2003); *Appl. Phys. Lett.* 82, 460 - 462 (2003), *Science* (submitted). Also supported by US Army Natick Soldier Systems Center.

Photonic Crystals Based on Periodic Arrays of Aligned Carbon Nanotubes

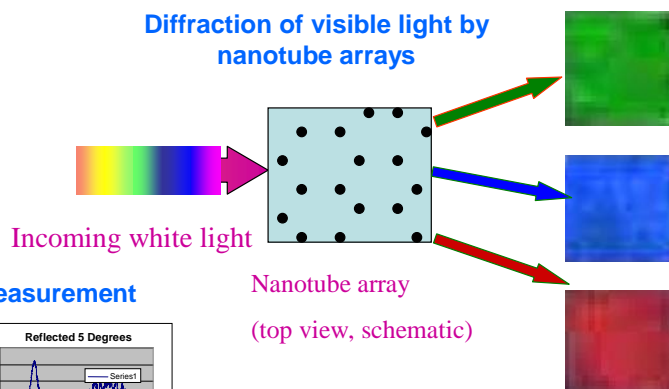
Z. F. Ren, Boston College

Large periodic arrays of well-aligned carbon nanotubes were fabricated inexpensively on Ni dots prepared via *self-assembled nanosphere lithography*. These structures show potential as 2D photonic band gap materials.

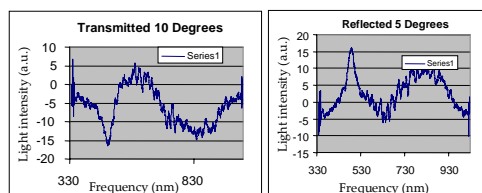
Aligned carbon nanotube arrays



Diffraction of visible light by nanotube arrays



Photonic band gap measurement



Boston College · Department of Physics

Kempa *et al.*, *NanoLetters* 3, 13 – 18 (2003).

Synthesis of Novel Zinc Oxide Nanostructures

Investigator: Z. F. Ren, Boston College

The synthesis of novel zinc oxide nanostructures including hierarchical structures with different symmetries, nanobridges, and nanowalls have been accomplished by a vapor transport and condensation technique. These hierarchical structures are different from the regular one-dimensional nanowires and nanotubes in the sense that they have secondary branches on the primary one-dimensional nanowires. The primary nanowires are indium oxide and the secondary nanostructures are zinc oxide. Scientifically, this work demonstrates the feasibility of joining two different nano-components. Technologically, these composite nanostructures have superior electrical and thermal conductivities due to their structural integrity. These nanostructures may find applications in field emission, photovoltaics, supercapacitors, fuel cells, and high strength and multifunctional nanocomposites. The work has been featured in the "Editor's Choice" section of Science, on the cover of the November 2002 issue of Nanoletters, and on the month of November of the American Chemical Society's Calendar for 2003, etc.

Reference: *NanoLetters* 2, 1287 - 1291 (2002); *NanoLetters* 3, 235 - 238 (2003); Also supported by The US Army Natick Soldier Systems Center.

Hierarchical ZnO Nanostructures

Z. F. Ren, Boston College


ZnO powder
+
In₂O₃ powder
+
Graphite powder

**1000 °C
vapor
deposition**

**In₂O₃
core wires**

**ZnO
branches**

Hierarchical ZnO Nanostructures



Boston College · Department of Physics

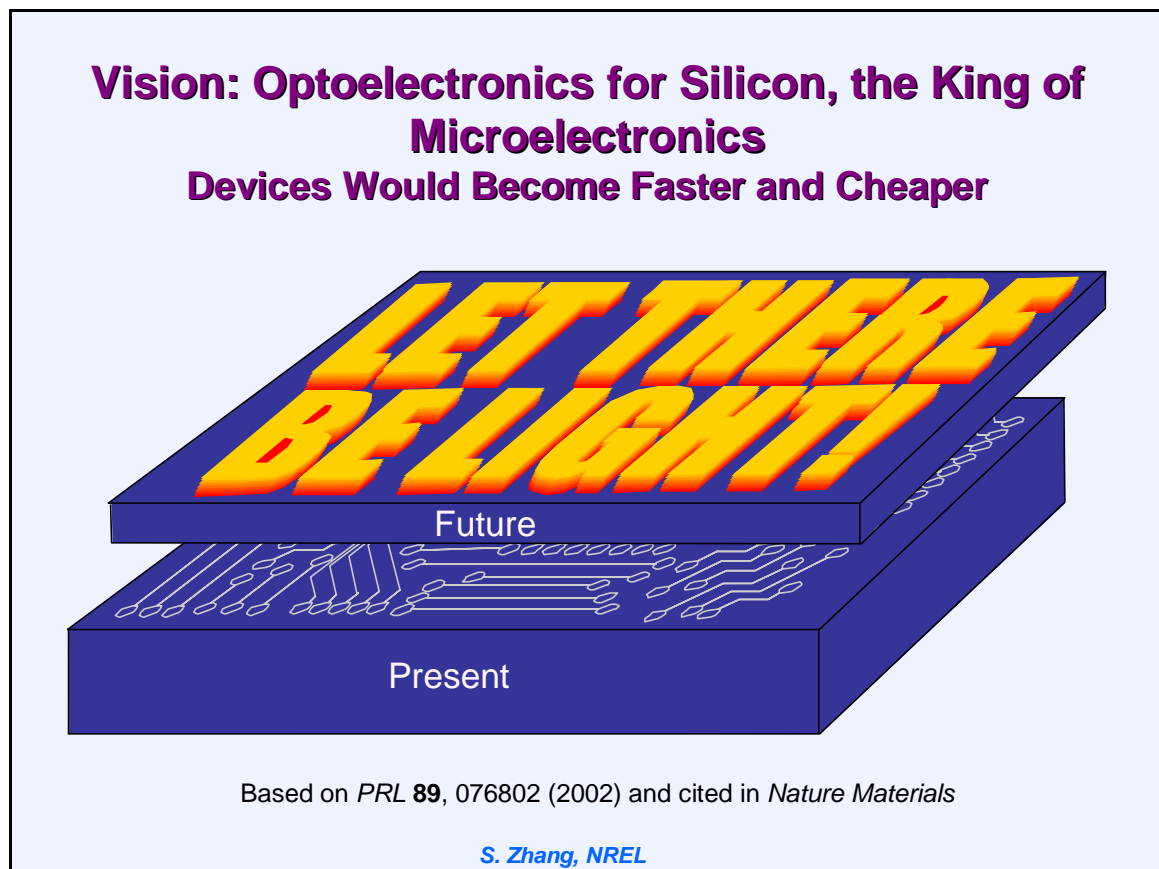
J. Y. Lao, et al. *Nano Letters* 2, 1287 – 1291 (2002)

Silicon: From Information Age to an Efficient Light Emitter?

Investigator: S. Zhang, National Renewable Energy Laboratory

Silicon is the bedrock on which the information age is built. But it is a notoriously poor light emitter. The holy grail of silicon technology is to make silicon an efficient light emitter so that digital information can be converted to light for the ultimate transmission speed across optical fiber networks. First-principles calculations showed that a novel impurity superlattice structure of thin-layer oxide could do precisely that by altering silicon electronic charge characteristics to couple directly to light. This breakthrough is likely to redirect the current research activities relying exclusively on “squeezing” light out of silicon by quantum size effects. By identifying the true origin of light emission, this research opens the door so that the light-emitting efficiency of silicon could be drastically enhanced. This is of considerable benefit to the microelectronics industry, and would enable the integration of optoelectronics into silicon-chip production to be easier, cheaper and more effective.

Reference: *Phys. Rev. Lett.* 89, 076802 (2002) and cited in Nature's materials update (article “Gap design” by Ed Gerstner on 8 August, 2002).



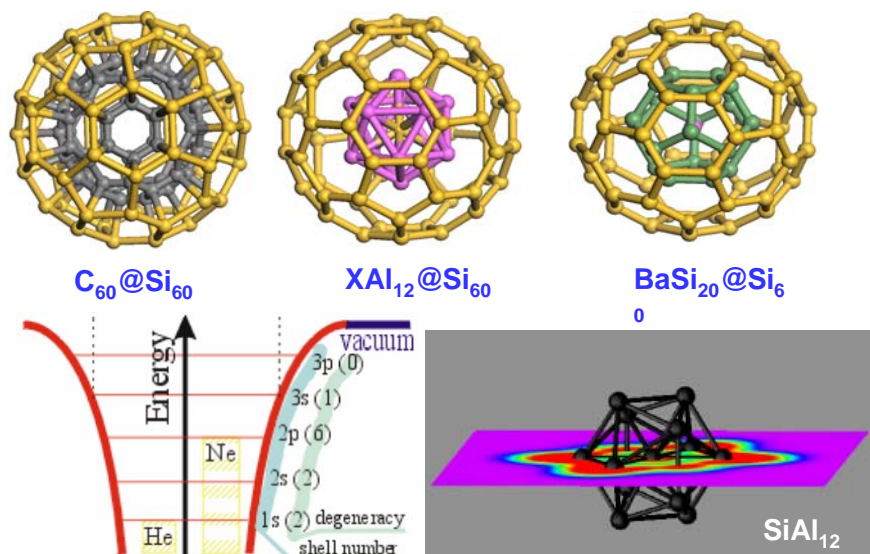
Russian Doll Model for the Stabilization of 60 Atom Silicon Cage Structure

Investigator: P. Jena, Virginia Commonwealth University

Although carbon and silicon belong to the same group of the periodic table, they have very different properties. While carbon forms graphitic, diamond and “fullerene” structures, silicon forms only tetrahedral bonds. Numerous attempts to stabilize the 60-atom silicon cluster in the shape of a 60 carbon atom “fullerene” have failed. First principles calculations, however, have now shown that a 60-atom silicon cluster can be stabilized by using a Russian doll model where a 60-atom silicon cluster encapsulates a smaller cluster, which in turn encapsulates an atom much the same way as having a doll inside a doll inside a doll. Compound magic clusters, such as a silicon atom inside 12 aluminum atoms and a barium atom inside 20 silicon atoms, were used as endohedral complexes. It was further shown that previous attempts to synthesize 60-atom silicon with 60-atom carbon as an endohedral complex failed because such a structure is energetically unfavorable due to the stretching of the silicon to silicon bonds. The ability to alter the traditional bonding characteristics of silicon at the nanoscale by incorporating metal atoms may have important implications for the design of novel silicon based electronic devices.

Reference: *Phys. Rev. Lett.* 90, 135503 (2003); selected for the April 14, 2003 issue of the Virtual Journal of Nanoscale Science & Technology.

Caged Metal Clusters Stabilize Silicon-based Fullerene Structures



Clusters can be used as super-atoms for novel nano structure design. The sp^3 bonding feature of Si atoms result in the instability of fullerene cage for Si_{60} cluster, which can be stabilized by encapsulation some small clusters: XAl_{12} (X = Si, Ge, Sn, Pb) and $BaSi_{20}$. However, C_{60} is too big in size for such a stabilization.

P. Jena, Virginia Commonwealth University

Understanding the Language of Corrosion

Investigator: H. Isaacs, Brookhaven National Laboratory

Does aluminum speak a different corrosion language than stainless steels? Electrical signals during corrosion have been used to monitor the presence and intensity of the corrosion process. These signals have been analyzed in terms of electrical noise and each stage of corrosion has its own signature. Earlier measurements showed that stainless steel has distinct and separate signals announcing the start and propagation of corrosion, such as pitting or stress corrosion cracking. However, it was uncertain that somewhat similar signatures from aluminum were due to the breakdown and repair of the protective nanometer-thick oxide film that protects all industrial metals. A new visualization technique revealed that the voice of corrosion arose from very different causes with different metals. Unlike stainless steel, aluminum is far more talkative with a greater vocabulary identifying various stages including oxide film breakdown, the staccato of pit growth, and the silence of passivity. Understanding the corrosion languages is essential to devise new procedures to improve the corrosion resistance of aluminum and other alloys. Corrosion damage presently costs the U. S. economy 4 % of the annual Gross National Product, and is a major deterrent to the performance limits, safety, and economy of both fossil and nuclear energy technologies.

Understanding the Language of Corrosion

H. S. Isaacs and K. Sasaki*

Material Science Department, Brookhaven National Laboratory, Upton, NY 11973

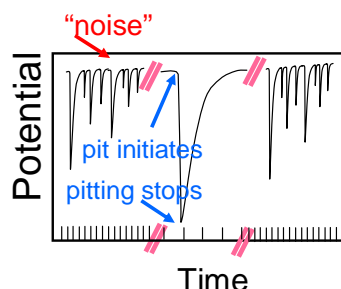
*Fontana Corrosion Center, The Ohio State University, Columbus, Ohio 43210

Electrochemical “noise” results from and is used to monitor corrosion but does the noise represent the same process for all metals and alloys?

New visualization technique answers the question!

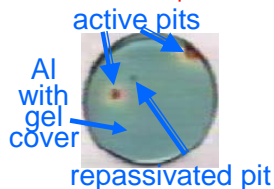
stainless steels

it had been shown
“noise” is caused when pits
initiate propagate and repassivate



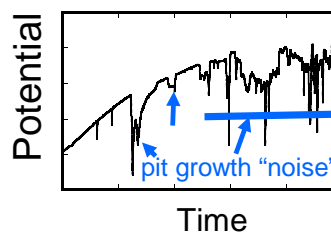
does aluminum
show the same
“noise” behavior
as stainless steel

new visual techniques
required development
using gels and pH
indicators to locate and
monitor for pits



aluminum and its alloys

“noise” is dominated by pit
growth processes not
initiation and repassivation

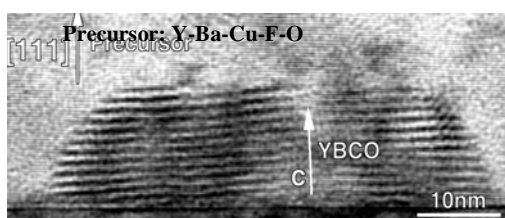


Newly Discovered Growth Process Enables Production of Thick Films of Superconducting YBCO That May Eventually Replace Costly Copper Conductors

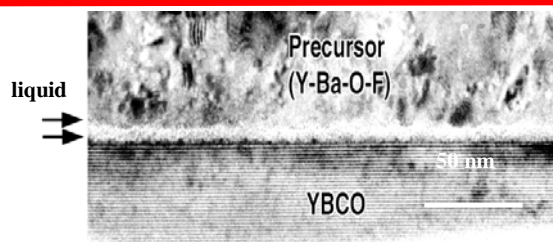
Investigator: M. Suenaga, Brookhaven National Laboratory

High temperature superconductors such as $\text{YBa}_2\text{Cu}_3\text{O}_7$ (YBCO) are able to carry very large electric currents without electrical resistance losses as in ordinary copper wires. To replace copper wires ubiquitously used in electric utility applications with YBCO would result in significant improvements in energy efficiency and consequential billion dollar savings. But growing sufficiently thick films of YBCO has not been feasible due to its complex growth mechanism. A new epitaxial liquid-assisted growth method, which involves a fluoride compound in precursor films, has been developed and the study yielded an understanding of the complex and unconventional growth process, which involves reactions of precursor films to form the desired compounds in several sequential steps. The new understanding has led to the successful growth of thick films of YBCO which is a necessary step toward the economic mass-production of superconducting wires of YBCO. Furthermore, this new understanding of epitaxial liquid-assisted growth may be extended to other technologically important oxides that are of critical importance in solid-state electronic devices.

Newly Discovered Growth Process Enables Production of Thick Films of Superconducting YBCO That May Replace Costly Copper Conductor



Epitaxial nucleation of a YBCO island on a substrate, from a precursor mixture, is a necessary first step during the initial fabrication process.



YBCO layer grows by epitaxial deposition of the compound from a liquid between the existing YBCO and the precursor.

- New epitaxial liquid-assisted growth method for YBCO was developed to yield an understanding of the complex and unconventional growth process.
- The understanding has led to the successful growth of thick films of YBCO needed for the economic mass-production of YBCO wires.

Brookhaven Science Associates
U.S. Department of Energy

M. Suenaga

BROOKHAVEN
NATIONAL LABORATORY

In-situ Observation of Structural Change in Giant Magnetocaloric Materials

Investigators: Gschneidner and Pecharsky, Ames Laboratory

The magnetic field induced structural transition in Gd_5Ge_4 , a giant magnetocaloric effect material, has been observed employing x-ray powder diffraction in a unique in-situ combination with high magnetic field. The structural transformation and the imaging of the shifting atoms were mapped out as a function of magnetic field at constant temperature, and as a function of temperature at constant magnetic field. The giant magnetocaloric effect arises from the amplification of a conventional magnetization mechanism by a substantial thermal effect of the magnetic field induced structural transition. The understanding of both the transformation and the mechanism of the giant magnetocaloric effect is vital for the future of magnetic refrigeration technology, which is poised to reduce the total US energy consumption by at least five percent and eliminate ozone-depleting and greenhouse chemicals. While temperature and pressure are common triggers of structural transitions, substantial magnetic field induced changes in the three-dimensional arrangement of atoms in the crystal lattice have been never directly visualized. Such new knowledge and understanding of the contributions from field induced magnetic and structural changes to the magnetocaloric effect pave the way to advanced materials, leading to improved cooling technologies.

